

LA-UR-14-26824

Approved for public release; distribution is unlimited.

Title: LANL Spectroscopic Modeling of Outputs

Author(s): Hakel, Peter
Timmermans, Eddy Marcel Elvire
Coe, Joshua Damon
Reynolds, James M.
Mozyrsky, Dima V.
Duffy, Leanne Delma
Nisoli, Cristiano
Sherrill, Manolo Edgar

Intended for: Report

Issued: 2014-08-30

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

LANL Spectroscopic Modeling of Outputs

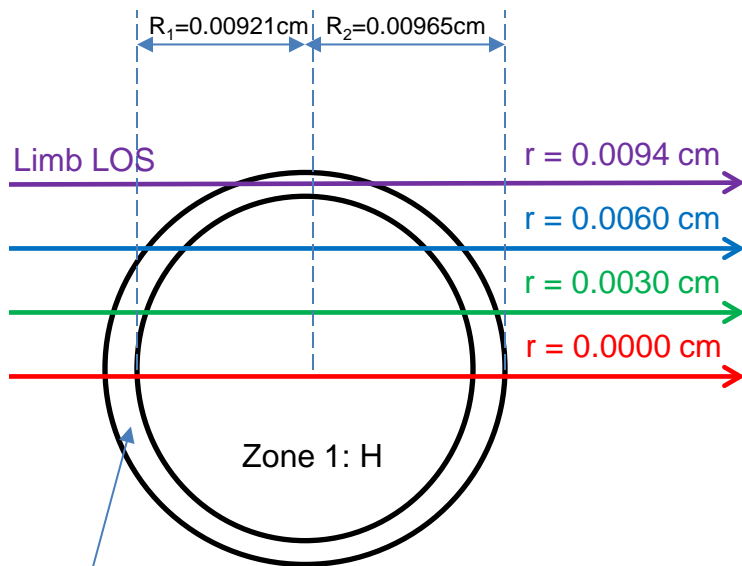
*Los Alamos is working on the further development of existing capabilities initially built for X-ray spectroscopy (postprocessing **RAGE** for the DIME project) and extending them to the infrared, visible, and ultraviolet regimes.*

To this end, LANL is expanding its area of expertise beyond atomic physics into molecular physics and opacities.

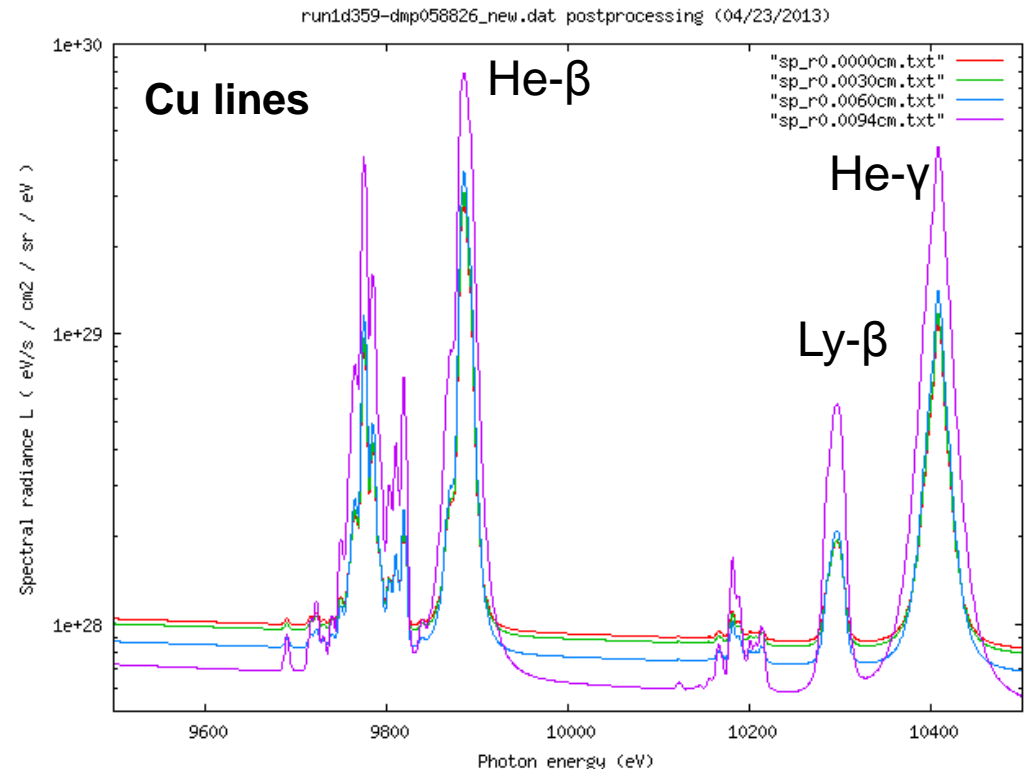
*Peter Hakel (XCP-5), Eddy Timmermans (T-4), Josh Coe (T-1),
Jim Reynolds (ISR-2, now Sandia Natl. Labs), Dima Mozyrsky (T-4),
Leanne Duffy (AOT-AE), Cristiano Nisoli (T-4), Manolo Sherrill (T-1)*

Starting point: postprocessing ICF simulations

FESTR model and code (currently 1-D, steady-state):
Finite-Element Spectroscopic Transport of Radiation



Zone 2: CD + 1% Cu



- Temperatures and densities (from RAGE) in each spatial zone are used by the ATOMIC¹ code to calculate mixed emissivities and opacities.
- The radiation transport equation is then solved to generate spectra.^{2,3}

[1] M.E. Sherrill et al., Physical Review E **76**, 056401 (2007).

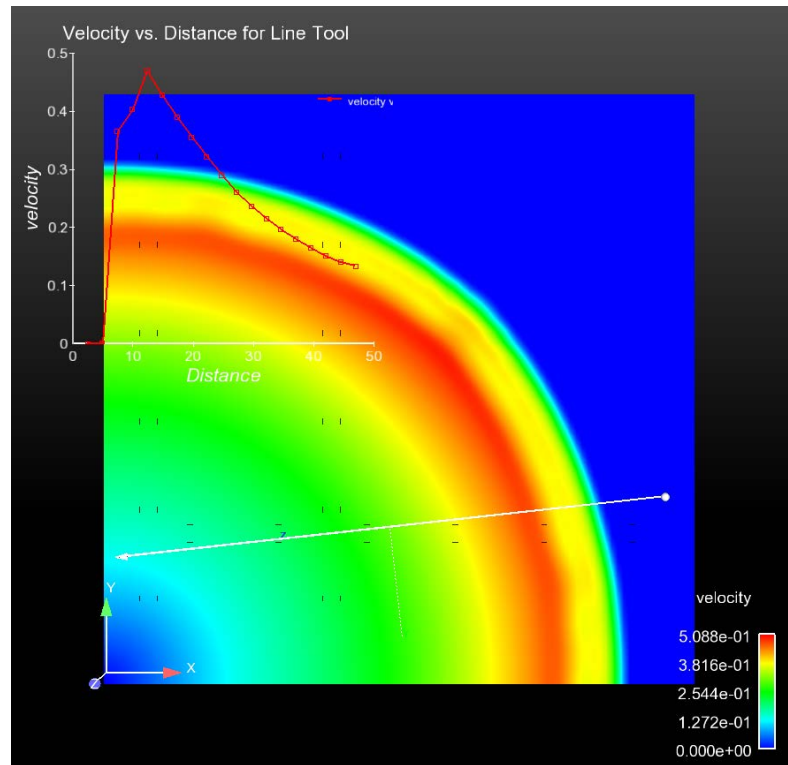
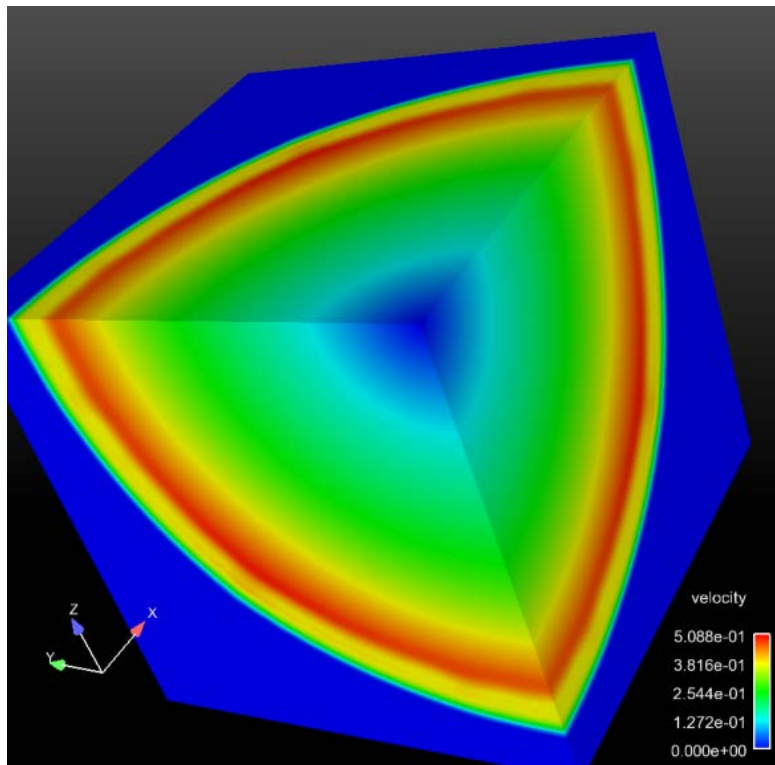
[2] P. Hakel et al., Physics of Plasmas **21**, 063306 (2014).

[3] J.A. Baumgaertel et al., Physics of Plasmas **21**, 052706 (2014).

UNCLASSIFIED

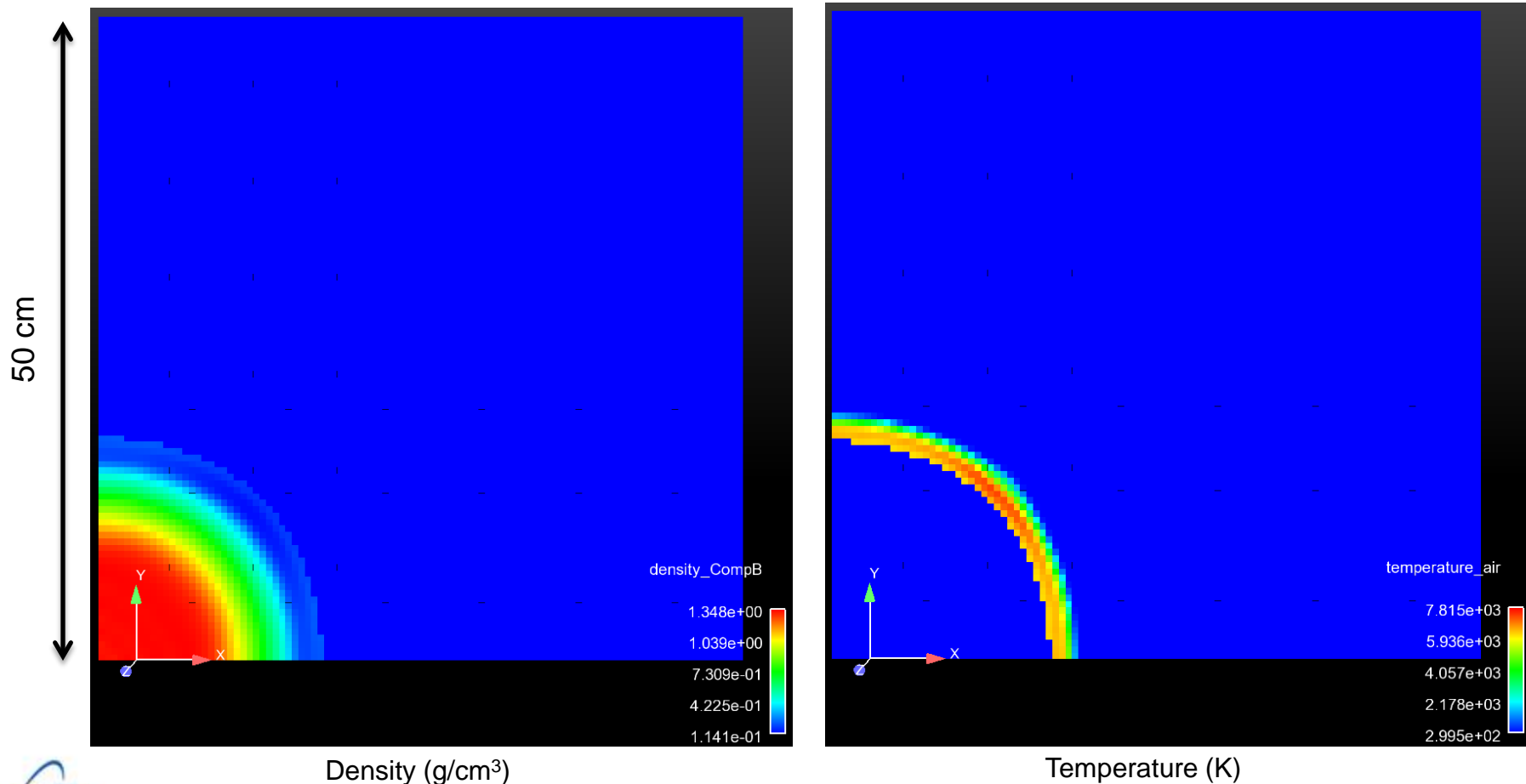
Spectral postprocessing of Pagosa simulations

- Relevant quantities (temperatures, densities, etc.) can be extracted from Pagosa dumps with EnSight visualization software, and saved into files.
- These files then can serve as input for spectral post-processing calculations.



Pagosa results were provided by Jim Reynolds.

Example of a Pagosa run modeling CompB



Pagosa results were provided by Jim Reynolds.

UNCLASSIFIED

Slide 4

Prototype model as input for FESTR



CompB:

$T = 1574 \text{ K}$

$\rho = 0.5 \text{ g/cm}^3$

thin shell, radius 15 cm

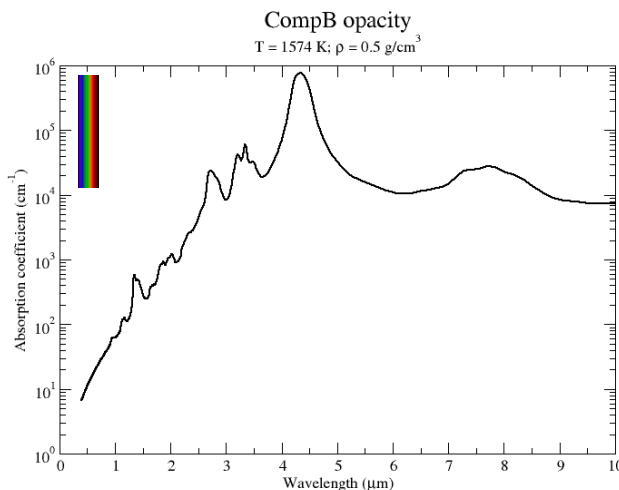
spherical geometry



Transport medium (air)

Source
("fireball")

Opacity data were provided by Eddy Timmermans with Josh Coe, Dima Mozyrsky, Leanne Duffy, and Cristiano Nisoli using the HITRAN molecular database.



Air:

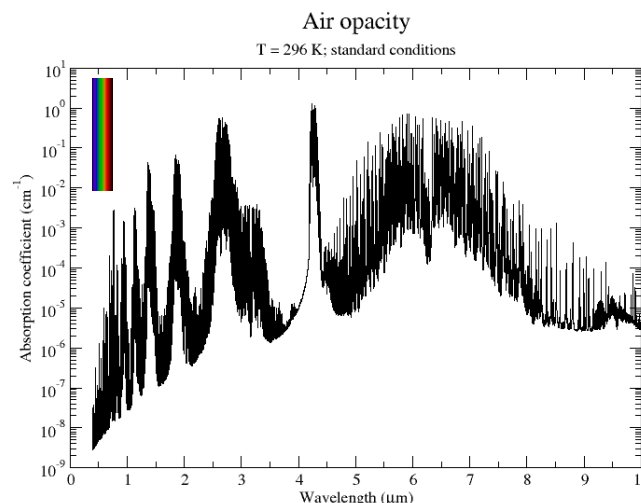
$T = 296 \text{ K}$

standard conditions

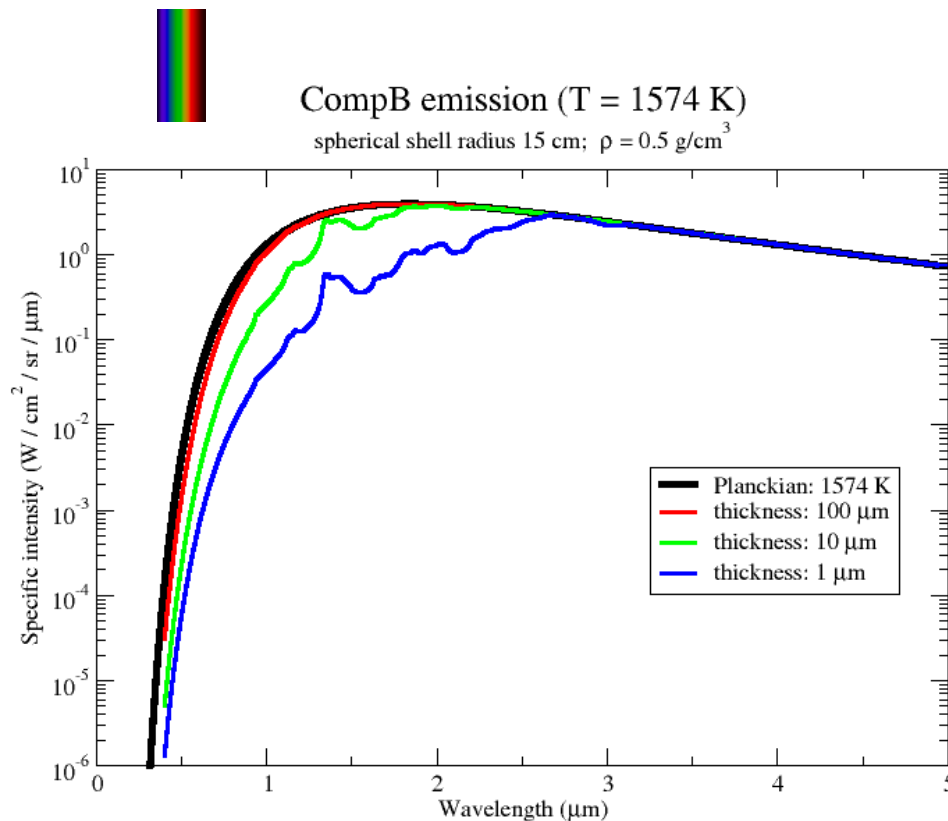
length 100 m

planar geometry

*Synthetic
spectrum
("detector")*



CompB self emission: three shell thicknesses

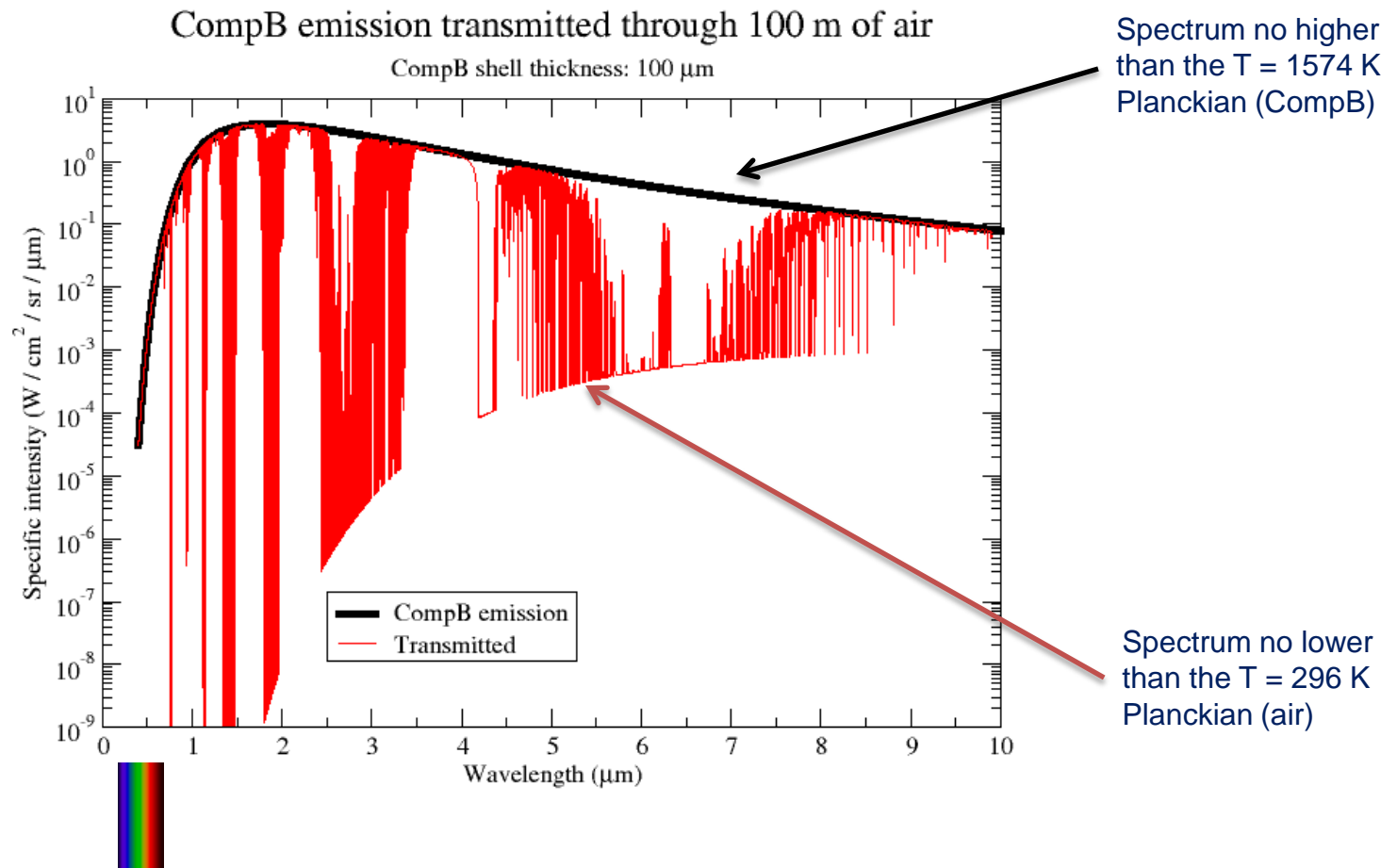


High opacity

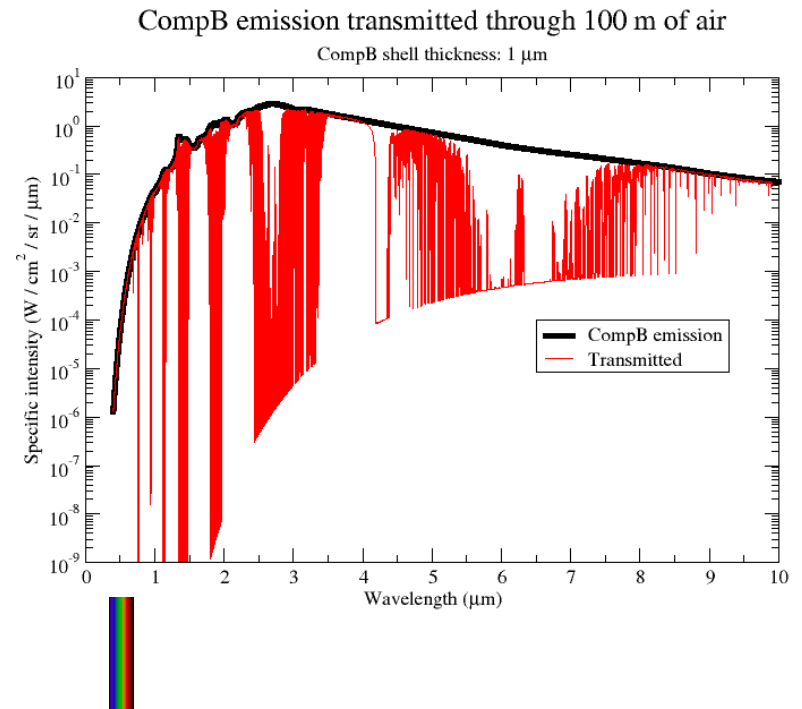
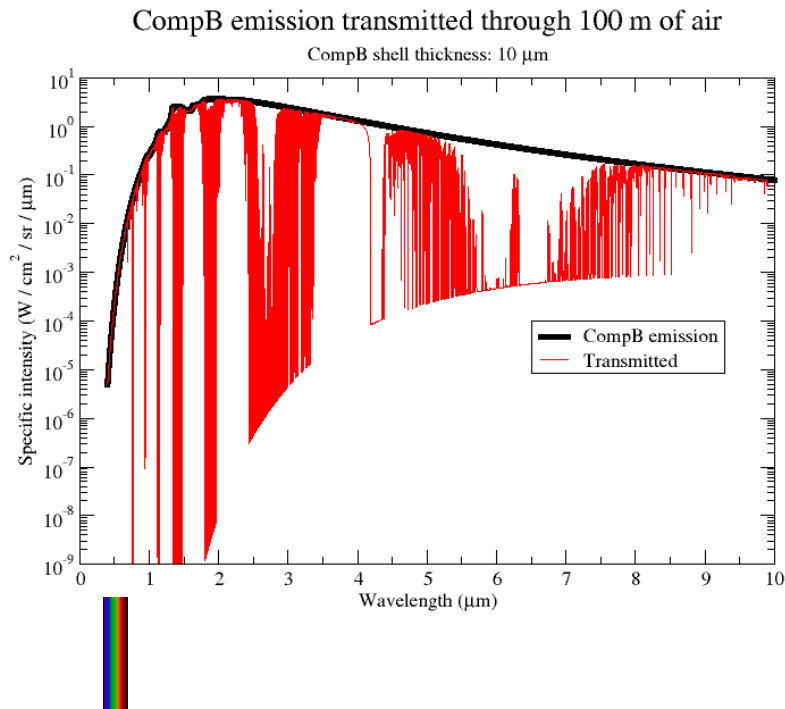


Blackbody spectrum:
i.e., the identity of the material
(encoded in its spectral characteristics)
can be obscured by the thermalization
of the output signal.

Transmission through air



Transmission through air



Summary

- A prototype model and code (FESTR) to calculate spectroscopic-quality outputs exists.
- FESTR currently handles 1-D and steady-state modeling; work is under way to generalize it.
- An effort to supply FESTR with opacities for molecular materials and their mixtures is ongoing.
- Hydrodynamic simulations (e.g., with Pagosa, RAGE, ...) can be performed to calculate the state of the relevant materials during output generation.
- Opacities need to access those regions of the parameter space suggested by the hydrodynamic simulations.